Stretched exponential relaxation of glasses and origin of the mixed alkali effect

Bauchy, Mathieu; Mauro, John C.; Smedskjær, Morten Mattrup

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Mathieu Bauchy *† [1], John Mauro [2], Morten Smedskjær [3]

[1] University of California, Los Angeles (UCLA) – United States
[2] Aalborg University – Denmark
[3] Penn State University – United States

Despite the dramatic increase in their viscosity as temperature decreases, some glasses are known to feature room-temperature relaxation. However, the structural origin of this phenomenon-known as the "thermometer effect"-remains unclear. Here, based on accelerated molecular dynamics simulations of alkali silicate glasses, we show that both enthalpy and volume follow some stretched exponential decay functions upon relaxation. However, we observe a bifurcation in their stretching exponents, with $\beta = 3/5$ and $3/7$ for enthalpy and volume relaxation, respectively-in agreement with Phillips' topological diffusion-trap model. Based on these results, we demonstrate that the thermometer effect is a manifestation of the mixed alkali effect. We show that relaxation is driven by the existence of stressed local structural instabilities in mixed alkali glasses. This driving force is found to be at a maximum when the concentrations of each alkali atom equal each other, which arises from a balance between the concentration of each alkali atom and the magnitude of the local stress that they experience.

Keywords: Molecular dynamics, relaxation, mixed alkali effect

*Speaker
†Corresponding author: bauchy@ucla.edu